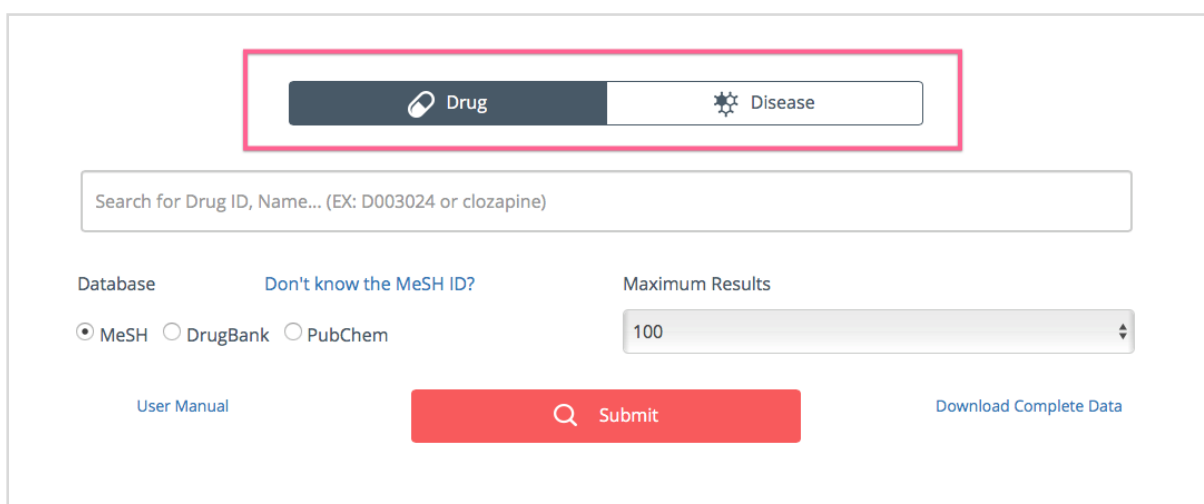


User Manual for SCMFDD

This user manual will walk you through the functions of web prediction tool for Drug-Disease Associations we provided [here](#).

1. Choose the type of the target

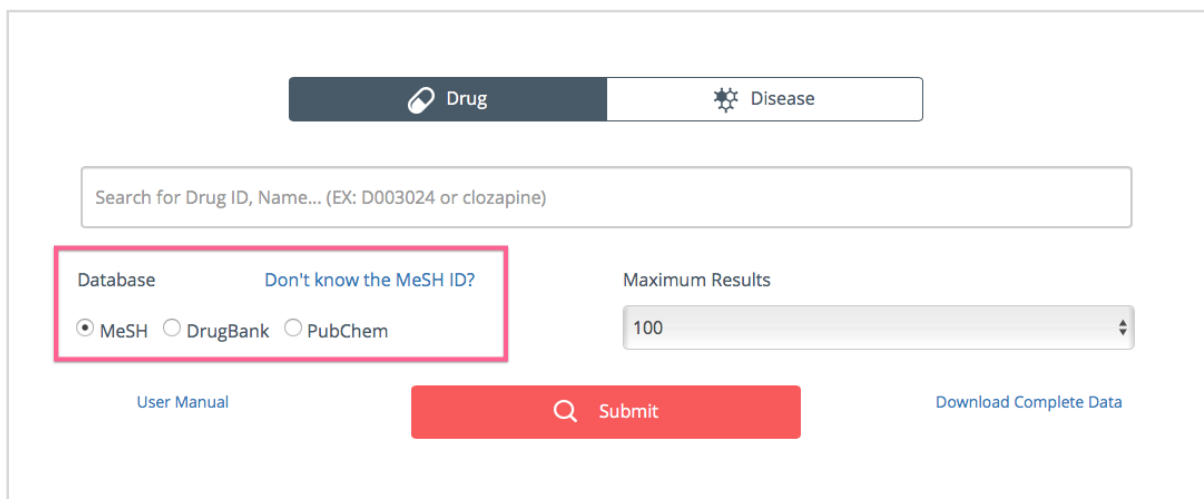
The tool we provided can be used to generate the predictions for certain drug or disease. For example, choose the **Drug** tab if you intend to get the result for a drug (like Clozapine or Aspirin).



The screenshot shows the SCMFDD web prediction tool interface. At the top, there are two tabs: 'Drug' (selected) and 'Disease'. Below the tabs is a search input field with the placeholder text 'Search for Drug ID, Name... (EX: D003024 or clozapine)'. Underneath the search field, there are three radio buttons for the database: 'MeSH' (selected), 'DrugBank', and 'PubChem'. To the right of the database options is a 'Maximum Results' dropdown menu set to '100'. At the bottom, there is a red 'Submit' button with a magnifying glass icon, a 'User Manual' link, and a 'Download Complete Data' link.

2. Specify a target

To get the predictions for the target you interested, you need to provide the identifier of it. For drug, we accept **MeSH ID**, **DrugBank ID** and **PubChem ID**, remember to choose the corresponding database option in order to get the correct result.



This screenshot is identical to the one above, but with a red box highlighting the 'Database' section. The 'MeSH' radio button is selected, and the text 'Don't know the MeSH ID?' is visible next to it. The 'Maximum Results' dropdown is also visible, set to '100'. The 'Submit' button, 'User Manual' link, and 'Download Complete Data' link are also present at the bottom.

For disease target, we currently recognize the MeSH ID only, so entering the MeSH ID for specified disease is all you need to do.

If you don't know any IDs of the target, you could go to the [MeSH](#), [DrugBank](#) and [PubChem](#) databases to search the IDs of your target using other features, or using the fuzzy search tool we developed by recognizing the name of the drug/disease.

3. Search for target by name (Optional)

If you are having trouble figuring out the IDs of the target, you can type the name of the target into the search bar and click the submit button, if the keyword you typed matches the record in our database, you would get the prediction result directly. However, in most cases, you only remember the synonyms or part of the full name of the target, under this circumstance, we provided the fuzzy search feature which allows you to check all the drugs or diseases which contained the keyword in its name or synonyms.

In the result table, keywords would be highlighted in the **Synonyms** column, you could click the IDs to view the external database to ensure that is which you are looking for. If you have confirmed one of the possible targets is exactly what you are interested in, click the link of the last column would redirect you to the predictions page.

Drug
Disease

tartrate

Database [Don't know the MeSH ID?](#)

MeSH
 DrugBank
 PubChem

[User Manual](#)

Maximum Results

100

Submit

[Download Complete Data](#)

Possible Drug Matching keyword: tartrate

Download CSV
Download PDF
Search:

Index	Synonyms	Drug MeSH ID	DrugBank ID	PubChem ID	Drug Name
1	vinorelbine tartrate	C030852	DB00361	44424639	vinorelbine
2	Acetylcholine L- Tartrate	D000109	DB03128	187	Acetylcholine
3	Carbamazepine L- Tartrate (4:1)	D002220	DB00564	2554	Carbamazepine
4	Choline Bi tartrate	D002794	DB00122	305	Choline
5	Disopyramide, D- Tartrate (1:1), (S)-Isomer	D004206	DB00280	3114	Disopyramide
6	Disopyramide, L- Tartrate (1:1), (R)-Isomer	D004206	DB00280	3114	Disopyramide
7	Disopyramide, L- Tartrate (1:1), (S)-Isomer	D004206	DB00280	3114	Disopyramide
8	Disopyramide, L- Tartrate (1:2), (+)-Isomer	D004206	DB00280	3114	Disopyramide

4. Inspect the prediction result

You would see the prediction result page after clicked the Submit button if you had entered the correct ID or name of the target, on top of the table, you can switch between 3 tab, **Prediction**, **Known Interaction** and **Visualization** section.

Name: Sleep Initiation and Maintenance Disorders | MeSH ID: [D007319](#)

Prediction Known Interaction Visualization

Download CSV Download PDF Search:

Index	Drug Name	Drug MeSH ID	DrugBank ID	PubChem ID	Score
1	Clozapine	D003024	DB00363	2818	1
2	Carbamazepine	D002220	DB00564	2554	0.6281
3	Amantadine	D000547	DB00915	2130	0.6041
4	Amphetamine	D000661	DB00182	3007	0.5434
5	Fluphenazine	D005476	DB00623	3372	0.5253
6	Cimetidine	D002927	DB00501	2756	0.509
7	Phenytoin	D010672	DB00252	1775	0.4994
8	Morphine	D009020	DB00295	5288826	0.4654

4.1 Prediction Section

In the **Prediction** section, here listed the prediction result for certain target sorted by the score, you can also sort the table by other field through clicking the header of the table. On the top left are the download functions, we provide CSV and PDF format to download the content in the table. On the top right is the Search input area, use it to search for specify keyword in the table. In the table, click the target name would redirect to the prediction result page for the clicked target, click other IDs would open the record for this target in other database.

Name: Sleep Initiation and Maintenance Disorders | MeSH ID: [D007319](#)

Prediction Known Interaction Visualization

Download CSV Download PDF Search:

Index	Drug Name	Drug MeSH ID	DrugBank ID	PubChem ID	Score
1	Clozapine	D003024	DB00363	2818	1
2	Carbamazepine	D002220	DB00564	2554	0.6281
3	Amantadine	D000547	DB00915	2130	0.6041
4	Amphetamine	D000661	DB00182	3007	0.5434
5	Fluphenazine	D005476	DB00623	3372	0.5253
6	Cimetidine	D002927	DB00501	2756	0.509
7	Phenytoin	D010672	DB00252	1775	0.4994
8	Morphine	D009020	DB00295	5288826	0.4654
9	Ketamine	D007649	DB01221	3821	0.4466
10	Maprotiline	D008376	DB00934	4011	0.4324

Show entries

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...
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4.2 Known Association Section

The **Known Association** section is very similar to the **Prediction** section, the main difference is that it doesn't have the **Score** column, for more detail please refer the 4.1 Prediction Section.

4.3 Visualization Section

In the **Visualization** section, you could inspect the result in a different way. Each node represents a drug or disease dependent on the category of the target you chose. Hover the mouse on the icon would display the detail for the node, click the node would redirect to the external database for more detail. Click the legend on the top would toggle the visibility of the selected links. On the top right are the download buttons, you could save the visualization as image or network file.

